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2018 FEARCE Development: A Robust and Accurate Engine Modeling Software

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Project Introduction

Research and development of **Fast, Easy, Accurate and Robust Continuum Engineering (FEARCE)**, formerly KIVA-hpFE) for turbulent reactive and multiphase flow, particularly as related to engine modeling, is relevant to the DOE Vehicle Technologies Office efforts at addressing national energy security. Less dependence on petroleum products leads to greater energy security. By Environmental Protection Agency standards, some vehicles are now reaching 42–50 mpg mark. These are conventional gasoline engines. With continued investment and research into new technical innovations, the potential exists to save more than 4 million barrels of oil per day or approximately \$200 to \$400 million per day. This would be a significant decrease in emissions and use of petroleum and a very large stimulus to the U.S. economy.

Better understanding of fuel injection and fuel–air mixing, thermodynamic combustion losses, and combustion/emission formation processes enhances our ability to minimize fuel use and unwanted emissions. Helping to accomplish this understanding, the **FEARCE** or KIVA development program is providing a state-of-the-art capability for accurately simulating combustion processes: to have a predictive methodology in a software helping industry and researchers not only meet national goals on fuel usage and emissions, but global goals. In addition, a predictive, robust, and accurate capability for simulating the engine combustion process helps to minimize time and labor for development of new engine technology.

Objectives

A main goal of the **FEARCE** or KIVA development project is to help provide better understanding of engine combustion processes in order to enhance the ability to minimize fuel use and unwanted emissions. The FEARCE development program is providing a state-of-the-art capability for accurately simulating combustion

processes and is providing a more predictive methodology than currently available in a software to supply industry and researchers a tool to help meet national goals on emissions and engine efficiencies. In addition, a predictive, robust, and accurate capability for simulating engine combustion processes helps to minimize time and labor for development of new engine technology. To meet these goals our program objectives are listed as follows:

Overall Objective

- Develop mathematical and computer algorithms and software for the advancement of speed, accuracy, robustness, and range of applicability of FEARCE, an internal engine combustion modeling software, to be a more predictive computer code. This is to be accomplished by employing higher-order, spatially accurate methods for reactive turbulent flow and more predictive spray injection, combined with a robust and accurate actuated parts simulation along with more appropriate turbulence modeling. In addition, we seek to understand the effect of heat transfer and the variation of temperatures on the internal combustion engine by creating easy to use numerical methods that eliminate all usual assumptions about such phenomena, such as assumed heat transfer processes at chamber and part boundaries. The code combines state-of-the-art chemical reaction simulators, such as Chemkin-Pro.
- To provide engine modeling software that is easier to maintain and is easier to add models to than the current KIVA codes, and reduce code development costs into the future via more modern code architecture. In addition, FEARCE is being developed to be a commercially available software, where DOE and LANL are doing the very difficult longer term research for better modeling software which is best done using National Lab type capabilities.
- To provide a software capable of producing fast turn-around times needed by industry. The code not only functions well on small computer platforms but addresses high performance computing aspects required for high-fidelity and more predictive solutions. These objectives require extensive use of high performance computing (HPC), thereby requiring our work to employ modern frameworks and methods that take advantage of computer resources very effectively; which FEARCE has accomplished by scaling to the size of the problem in a super-linear manner, the holy grail of HPC.

Fiscal Year 2018 Objectives

- Develop a 4-valve Direct Injection, Spark Ignition (DISI) engine system for validation of FEARCE.
- Validation progress of FEARCE on experimental data of the 4-valve DISI engine. Collaborating with Dr. Magnus Solberg of SNL on the DISI setup and experimental data.
- Construct systems to use ChemKin II and III and ChemKin-Pro reactive chemistry softwares.
- Continue spray model development, for both predictive spray break-up and subsequent droplet transport and fate. Implement the KH-RT spray model and perform validation against data stored on the ECN website from various experimentalists.
- Developed faster linear solver system by implementing a multigrid solution system of linear equations that better our current implicit solutions methods by more than a factor of two.
 - Invented a method for implementing Message Passing Interface (MPI) for today's and future platforms (Waters and Carrington 2016) that is super-linear.
- Begin the process of commercialization of FEARCE.

Approach

Our approach is founded in designing, inventing, and developing new modeling methods and software. The design is a finite element method (FEM). Many beneficial and salient attributes of the software stems from the FEM formulation. We invented and developed the following systems to date (details are provided in the referenced publications).

- Developed the FEM predictor–corrector scheme projection method for high accuracy and all the benefits the FEM system brings to computational fluid dynamics (CFD) modeling of engines (Carrington 2009, Carrington et al. 2014)
- Developed the hp-adaptive system for higher order accuracy where ‘h-adaptive’ is automatic grid refinement, and ‘p-adaptive’ is higher order approximation as driven by the error measure of the simulation (Carrington et al. 2014)
- Invented the local-arbitrary Lagrangian–Eulerian (ALE) method for moving bodies (Carrington, et al. 2018)
 - *Invented a moving marker system to track any chosen interfaces and reconstruct intersected elements to match the interface*
- Developed immersed boundary methods for moving bodies (Waters and Carrington, 2018)
- Developed new dynamic large eddy simulation (LES), specifically designed for wall bounded flows (Waters et al. 2016)
 - *Self-damping turbulence at the walls negates the need for a law-of-the-wall system*
- Invented and developed volume of fluid (VOF) methods in FEM for true multi-phase compressible flow
 - *To fully represent the spray break-up process, to have predictive spray modeling (Waters et al. 2017).*
- Developed a fast linear solver system
 - Developed parallel solution method (Waters and Carrington 2016)
 - Delivering 30× speed-up over serial code given the same problem and settings
 - Implicit solutions methods for 10× speed-up over serial parallel for an overall 300× speed-up
 - *Added Trilinos Multigrid matrix solution further improving solution speed and parallel scaling by order of magnitude (8x) over Implicit Beam-Warming system in FEARCE (that delivers 300x) for a total of 2400x speed-up over explicit serial version*
 - *Delivers superliner scalability*
- Invented a method for implementing Message Passing Interface (MPI) for today’s and future platforms (Waters and Carrington 2016)

We are building models and code so that they meet all the objectives in an easy to maintain software that easily handles addition of others’ submodels. Careful verification and validation of the methods and code is required. The development of this technology utilizes many areas of expertise of multi-species turbulent reactive flow modeling with liquid sprays, modeling of immersed moving bodies, and the extensive numerical methods for the solution of the model and governing equations developed in the software.

Results

Our efforts this year continue to push toward a comprehensive tool for the future with the accomplishment of more grid generation improvements, validation of immersed moving part including 4-valve Direct Injected Spark Ignition (DISI) engine, the KH-RT spray model, and an algebraic multigrid linear equation solver implementation for even greater computational speed. We’ve also begun the process of commercializing the software to be able to fully support industries and researchers requirements of a simulation software.

Grid Generation

- In conjunction with Program Development Company who developed GridPro, we are working on providing high quality grids for the engine system with an eye toward ease of use. The overset parts system used in the moving parts algorithm allows for easy grid generation of the cylinders and ports, with the spark and injector modules easily inserted. The piston and valves surfaces simply are also inserted by overlaying their surface representations after a quality grid is automatically generated.
- The overset gridding greatly simplifies the gridding process, removing the need to work around immersed bodies employed in traditional gridding methods. The injector and spark systems are built separately with the idea of making various types of injectors and spark plug modules that are simply connected to the engine cylinder grid. It cannot be overstated: a quality grid is needed to produce reliable simulations. Gridding is a major component of CFD, where we seek to provide that quality with a minimum of labor.

Engine Simulation and Continued Validation of Immersed Moving Parts for the Engine system

- Developed immersed boundary method and developing the immersed finite element methods for moving bodies using FEARCE's surface marker system
 - Partially based on methods used in our local- ALE system for moving bodies
 - The moving marker system utilizes track moving boundary interfaces (Carrington et al. 2018).
 - Immersed boundary employs interpolation and projection of nearest nodal values normal to the surface. Immersed FEM utilizes the shape or basis functions for interpolation and a projection system to place a point along the normal to the surface from which the nearest node is projected, the fluid's motion and thermodynamic state is calculated.
 - A four-valve engine test case is functioning as shown in Figure 1 using the immersed boundary methods, showing turbulent flow structures (by vorticity).

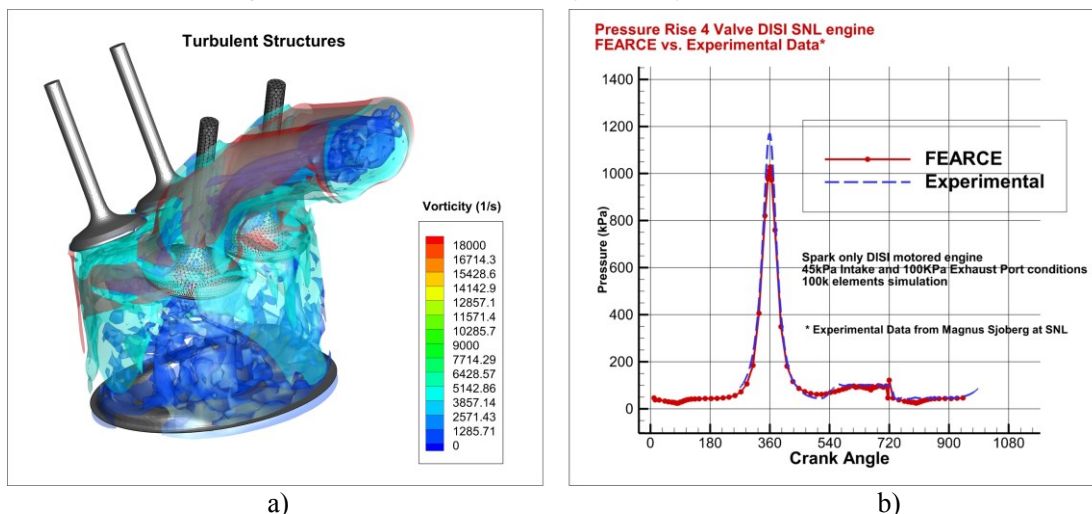


Figure 1 - 4-valve DISI engine, a) turbulent structures shown by magnitude of vorticity (1/s) during intake, b) Pressure Rise as a function crank angle (CA) as compared to experimental data

Spray Modeling

Implemented the Kelvin Helmholtz – Rayleigh Taylor (KH-RT) spray model into FEARCE. Tests have been conducted on Spray A and Spray G Engine Combustion Network (ECN) test cases to date with the following results. The KH-RT spray model (Reitz 1987) for the Spray A case is injection of diesel into quiescent nitrogen at 2.2 MPa is shown in Figure 2. Figure 2a, shows the droplets at 2 μ s. Figure 2b shows the penetration (mass moment distribution) of the spray droplets over time compared with experimental data from ECN.

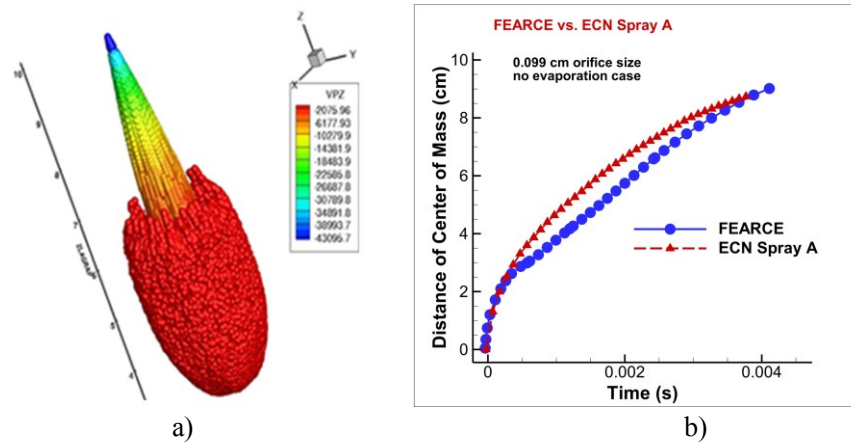


Figure 2 - The ECN Spray A case: injection of diesel in quiescent nitrogen at 2.2 MPa, KH-RT spray model, b) the penetration depth of the spray compared to ECN experimental data.

- Developing a system for fully representing the injection process from our current predictive spray break-up process using Volume of Fluids shown in Figure 3; handing off the predicted spray break-up into ligaments and subsequent droplet transport modeling and evaporation allowing true spray break-up transition to the Lagrangian particle and Rayleigh–Taylor secondary break-up systems, thereby producing more accurate engineering modeling for the injection system. Figure 3 shows liquid being injected into air at 3 bar through an orifice of 0.01-mm diameter early in time. The break-up length where the wave instabilities are large enough to cause ligamentation is five orifice diameters downstream of inlet, which is near the results obtained by Direct Numerical Simulation (DNS) as reported in Waters et al. (2017).

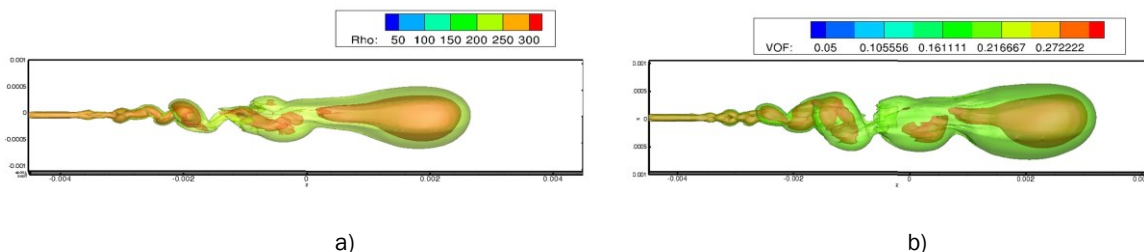


Figure 3 - Multiphase flow simulation with VOF method, gasoline injected into quiescent air at 3 bar. (a) Gasoline jet primary break-up into ligaments and (b) primary break-up and w-component of velocity of air showing recirculation.

Computational Efficiency

Continued work on parallel solution method and reducing wall clock time by adding the Trilinos Multigrid preconditioning. Previously we had developed a 10 \times speed-up with the implicit solve related to increased time step size. Additionally, we produced a 30 \times speed-up over the serial version with the implementation of shared-node FEM system that reduces communication cost and produces a super-linear scaling for an over 300 \times speed-up (Waters and Carrington 2016). Installed systems to access Trilinos solver package where the multigrid preconditioning is providing about 8 \times speed-up for a total of 2400 \times speed-up over the serial version of FEARCE. Multigrid improves the already good parallel scaling when running on a large number

of processors as. Keeping in mind, that the parallel version of FEARCE is significantly faster than KIVA-4mpi the parallel version of KIVA-4, significant strides have been made at the speed of solution.

- Delivering superlinear scalability as was demonstrated in Waters and Carrington 2016, in a strong scaling experiment on a standard CFD benchmark problems such as the backward-facing step or flow over a cylinder. Shown in Figure 4 is the scaling of FEARCE's algorithm (without special linear equation solver treatments such as preconditioning or multigrid) besting the ideal linear scaling.
- Implemented access to the Algebraic Multigrid Preconditioning and linear equation solvers from Trilinos (<https://trilinos.org/>).
 - Improved wall clock times by a factor of 8 over our original 300x speed-up beyond 2400x speed-up over our explicit serial solver as shown in Figure 5. Now encroaching on exceptional HPC performance. Note that optimal performance usually requires some domain distribution alteration, not simply the doubling shown in the scaling analysis Figure 4 and 5.
 - Further gains in the wall-clock times are expected for the super-linear system by employing greater vectorization and use of GPU's (use of Kukkos with Trilinos).
- Significant to note that FEARCE requires far fewer elements to achieve the same accuracy as older KIVA codes, allowing for must faster solution on same resolution with higher accuracy. This is the idea of HPC computing, getting the most solution accuracy and speed from the least amount of computational work, utilizing the least of a computer and getting better accuracy, allowing for high resolution systems having extremely good accuracy.
- FEARCE produces better accuracy than previous codes and on coarser grids. Hence, the new code is capable of being faster on the same resolution as old codes, but is more accurate even on less resolved problems, providing additional advantages. Previous reports show ever increasing computational speed versus KIVA-4mpi.

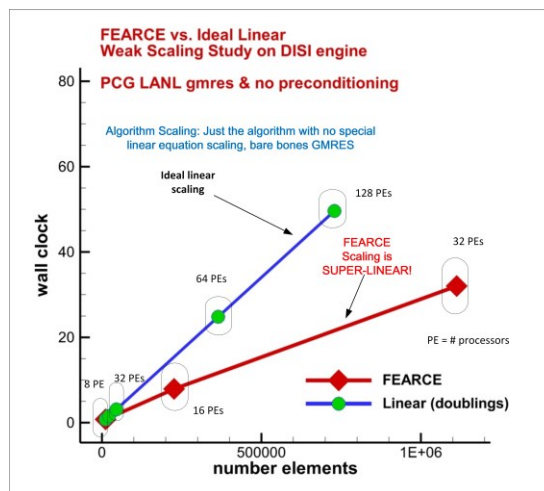


Figure 4 – FEARCE's super-linear algorithm scaling versus the ideal scaling curve.

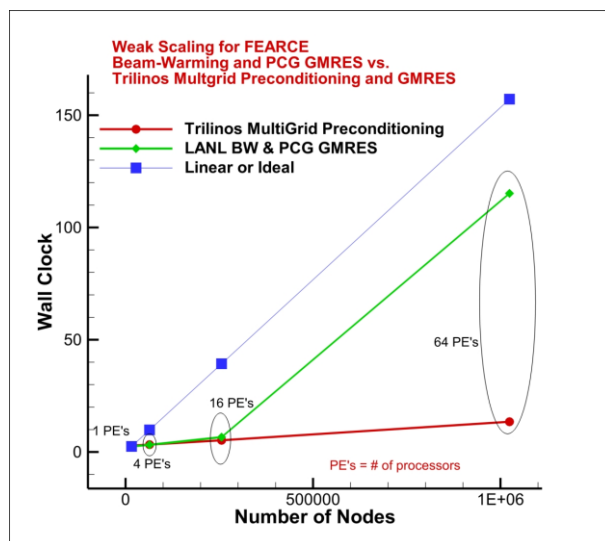


Figure 5 – FEARCE’s Beam-Warming system versus use of Trilinos Multigrid preconditioned GMRES, a weak scaling study

Conclusions

The KIVA development program at Los Alamos National Laboratory is nearing the objective of having a robust state-of-the-art CFD software for turbulent reactive flow, particularly well-suited for combustion modeling in engines or machines where immersed moving boundaries are involved, all with an eye toward solutions produced on quality grids created with a minimal amount of labor.

- Fast grid generation: computer-aided drawing to CFD grid in nearly a single step
- 4-valve DISI engine experimental data used to validate the robust moving immersed FEM method
- KH-RT spray model added to the code with validation ongoing via the ECN test cases
 - Spray A case with KH-RT for validation
 - Spray G cases with evaporation proceeding
- Predictive spray modeling with the addition of VOF method
 - Developing transition to Lagrangian particle transport from predictive spray break-up for engineering type simulations
- Highly scalable parallel solution system, with multigrid preconditioning producing nearly perfect scaling, 2400 times faster than serial version of FEARCE, 8 times faster than just the superlinear FEARCE and only gmres Krylov linear equation solve.
 - Researching Exascale possibilities by using vectorizable Cuda friendly sections of code for GPU processing nested into the MPI parallel framework.
- ChemKin II/III and also Chemkin-Pro added for faster, larger, and more robust reactive chemistry.

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Acronyms, Abbreviations, Symbols, and Units

KH-RT	Kelvin Helmholtz – Raleigh Taylor
FEM	Finite Element Method
VOF	Volume of Fluids
ECN	Engine Combustion Network
LES	Large Eddy Simulation